



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 148073

TO: Rei-Tsang Shiao
Location: 5a10 / 5c18
Thursday, March 24, 2005
Art Unit: 1626
Phone: 571-272-0707
Serial Number: 10 / 653618 *88*

From: Jan Delaval
Location: Biotech-Chem Library
Remsen 1a51
Phone: 571-272-22504
jan.delaval@uspto.gov

Search Notes

Jan. Deland
for search

Access DB: 148015

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Robby) Shiao Examiner #: 79521 Date: 3/17/05
Art Unit: 1626 Phone Number: 2-0107 Serial Number: 19653, 688
Mail Box and Bldg/Room Location: 5A12/sc 78 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

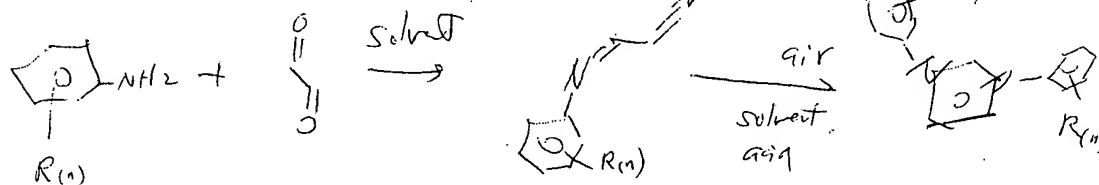
Title of invention: Synthesis of 1,3-disubstituted

Inventors (please provide full names): Nolan

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

2. Search a process for making imidazolium salt
by: (see Diagram D) see claim 1, 2/18



* R is sub, i.e.
alkyl

STAFF USE ONLY

STAFF USE ONLY		Type of Search	Vendors and cost where applicable
Searcher: <u>Jan</u>	NA Sequence (#) _____	STN <input checked="" type="checkbox"/>	
Searcher Phone #: <u>2-504</u>	AA Sequence (#) _____	Dialog _____	
Searcher Location: _____	Structure (#) <input checked="" type="checkbox"/>	Questel/Orbit _____	
Date Searcher Picked Up: <u>3/24/05</u>	Bibliographic _____	Dr. Link _____	
Date Completed: <u>3/24/05</u>	Litigation _____	Lexis/Nexis _____	
Searcher Prep: Review Time _____	Fulltext _____	Sequence Systems _____	
Clerical Prep: me: <u>15</u>	Patent Family _____	WWW/Internet _____	
Online Time: <u>445</u>	Other _____	Other (specify) _____	

=> d his

(FILE 'HCAPLUS' ENTERED AT 14:12:00 ON 24 MAR 2005)

DEL HIS
E NOLAN S/AU
L1 75 S E3,E8,E30,E32,E35,E37
L2 5 S L1 AND ?IMIDAZOL?
L3 1 S L2 AND 1 3 DISUBSTITUTED
L4 11 S 1 3 BIS 2 6 DIISOPROPYLPHENYL IMIDAZOLIUM CHLORIDE
L5 14 S 1 3 BIS 2 6 DIISOPROPYLPHENYL IMIDAZOLIUM?
L6 2 S L2 AND ?DIISOPROPYL?
L7 3 S L2 AND (1 3 OR 2 6)
L8 1 S L3 AND L6,L7
L9 3 S L6-L8
L10 2 S L9 AND BIS
SEL RN

FILE 'REGISTRY' ENTERED AT 15:01:24 ON 24 MAR 2005

L11 11 S E1-E11
L12 1 S L11 AND NCNC2/ES AND CL
L13 1 S 286014-24-2
L14 10 S 286014-24-2/CRN
L15 1 S L14 AND I
L16 2 S L12,L15
L17 1 S L11 AND C2H2O2
L18 1 S L11 AND C12H19N
L19 1 S L11 AND C26H36N2
E PARAFORMALDEHYDE/CN
L20 1 S E3
E HYDROCHLORIC ACID/CN
L21 1 S E3
E BF4H/MF
L22 1 S 14874-70-5
E TETRAFLUOROBOR/CN
E F6P/MF
L23 3 S E3
L24 7 S L11 NOT CCS/CI

FILE 'HCAPLUS' ENTERED AT 15:31:22 ON 24 MAR 2005

L25 695 S ?DIAZABUTADIEN?
L26 0 S L1 AND L25

FILE 'REGISTRY' ENTERED AT 15:32:31 ON 24 MAR 2005

L27 5 S (METHANOL OR ETHYL ACETATE OR ETHANOL OR TETRAHYDROFURAN OR T
E C20H24N2/MF
L28 153 S E3 AND 46.150.18/RID AND 2/NR
L29 3 S L28 AND BENZENAMINE AND ETHANEDIYLIDENE BIS
L30 2 S L29 AND TRIMETHYL
L31 1 S DIOXANE/CN
L32 1554 S 123-91-1/CRN
L33 5 S L32 AND CLH
L34 2 S L33 AND 2/NC
L35 3 S L11 AND NCNC2/ES NOT L12,L13
L36 1 S L35 AND C27H36N2
L37 1 S 244187-81-3/CRN
L38 1 S METHANOL/CN
L39 1 S ETHYL ACETATE/CN

FILE 'HCAPLUS' ENTERED AT 15:37:56 ON 24 MAR 2005

L40 6694 S L17
L41 11213 S GLYOXAL
L42 528 S ETHANEDIAL
L43 18 S GLYOXAZAL

L44 36 S GLYOXYLALDEHYDE
L45 12111 S L40-L44
L46 33 S L30
L47 61 S L16
L48 4 S L45 AND L47
L49 2 S L46 AND L47
L50 2 S L48 AND L49
L51 5 S L16 (L) PREP+NT/RL
L52 3 S L51 AND L45,L46
L53 1 S L1 AND L47
L54 3 S L52,L53
L55 0 S L54 AND L31,L34,L27
L56 0 S L54 AND L20-L23
L57 0 S L54 AND L27
L58 2 S L37
L59 0 S L37(L) PREP/RL
L60 8 S L10,L54,L58,L51
L61 3 S L60 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L62 4 S L10,L61

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 15:43:53 ON 24 MAR 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 24 Mar 2005 VOL 142 ISS 13

FILE LAST UPDATED: 23 Mar 2005 (20050323/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l62 all hitstr tot

L62 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:183602 HCAPLUS
ED Entered STN: 11 Mar 2003
TI Synthesis of 1,3-disubstituted
imidazolium salts
AU Kelly, Roy A., III; Sommer, William; Nolan, S. P.
CS Department of Chemistry, University of New Orleans, New Orleans, LA,
70148, USA
SO Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United
States, March 23-27, 2003 (2003), INOR-559 Publisher: American Chemical
Society, Washington, D. C.
CODEN: 69DSA4
DT Conference; Meeting Abstract
LA English
AB Imidazolium salts are the immediate precursors to N-heterocyclic
carbenes (NHC) yet a simple, general synthetic route to a wide variety of
imidazolium salt is not yet available. Such a straightforward

route is described for two specific members of this family of ligand precursor: **1,3-Bis(2,4,6-trimethylphenyl)imidazolium chloride** (IMes-HCl) and **1,3-Bis(2,6-diisopropylphenyl)imidazolium chloride** (IPr-HCl). The procedure appears general and similar protocols can be used to isolate various **imidazolium** salts. These and related NHC have been used in the synthesis of numerous palladium complexes. The general synthetic route to NHC precursors and the complexation to various metal centers will be discussed.

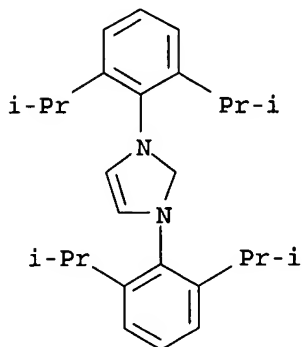
✓ L62 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:656855 HCAPLUS
 DN 133:362823
 ED Entered STN: 20 Sep 2000
 TI A sterically demanding nucleophilic carbene: **1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene**. Thermochemistry and catalytic application in olefin metathesis
 AU Jafarpour, L.; Stevens, E. D.; Nolan, S. P.
 CS Department of Chemistry, University of New Orleans, New Orleans, LA, 70148, USA
 SO Journal of Organometallic Chemistry (2000), 606(1), 49-54
 CODEN: JORCAI; ISSN: 0022-328X
 PB Elsevier Science S.A.
 DT Journal
 LA English
 CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 75
 OS CASREACT 133:362823
 AB The sterically demanding nucleophilic carbene ligand **1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene** (IPr, 4) has been synthesized. The reaction of [Cp*RuCl]₄ (5; Cp* = η⁵-C₅Me₅) with this ligand affords a coordinatively unsatd. Cp*Ru(IPr)Cl (6) complex. Solution calorimetric results in this system provide information concerning the electron donor properties of the carbene ligand. Steric parameters associated with this ligand are determined from the x-ray crystal structure study. The carbene ligand reacts with RuCl₂(:C(H)Ph)(PCy₃)₂ to yield a mixed carbene-phosphine ruthenium complex RuCl₂(:C(H)Ph)(IPr)(PCy₃) (9). A single-crystal x-ray diffraction study has been performed on 9. The thermal stability of 9 has been studied at 60° and its catalytic activity has been evaluated for the ring closing metathesis of di-Et diallylmalonate.
 ST sterically demanding nucleophilic carbene isopropylphenyl **imidazolylidene** ruthenium complex prepn; thermochem catalysis olefin metathesis isopropylphenyl **imidazolylidene** ruthenium complex; catalyst ring closing metathesis diallylmalonate isopropylphenyl **imidazolylidene** ruthenium complex; crystal mol structure isopropylphenyl **imidazolylidene** nucleophilic carbene ruthenium complex
 IT Cyclization catalysts
 (metathesis; preparation of sterically demanding nucleophilic carbene **bis(diisopropylphenyl)imidazolylidene** ruthenium complexes as)
 IT Crystal structure
 Molecular structure
 (of sterically demanding nucleophilic carbene **bis(diisopropylphenyl)imidazolylidene** ruthenium complexes)
 IT 3195-24-2, Diethyl diallylmalonate
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (**bis(diisopropylphenyl)imidazolylidene** ruthenium complex catalyzed ring closing metathesis of)

- IT 307519-47-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)
- IT 74663-75-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and cyclization of)
- IT 250285-32-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and neutralization of)
- IT 244187-81-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and reaction with ruthenium complexes)
- IT 21622-00-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 307519-48-8P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation);
PREP (Preparation); USES (Uses)
(preparation, crystal structure, and ring closing metathesis catalysis of
diallylmalonate with)
- IT 113860-07-4, Tetrakis(chloro(η^5 -pentamethylcyclopentadienyl)ruthenium)
172222-30-9, (Benzylidene)dichlorobis(tricyclohexylphosphine)ruthenium
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with bis(diisopropylphenyl)
imidazolyliidene as sterically demanding nucleophilic carbene)
- IT 107-22-2, Glyoxal
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with diisopropylaniline)
- IT 24544-04-5, 2,6-Diisopropylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with glyoxal)

RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Ackermann, L; Tetrahedron Lett 1999, V40, P4787 HCAPLUS
- (2) Anon; private communication from AJ Arduengo III
- (3) Arduengo, A; US 5077414 1991 HCAPLUS
- (4) Arduengo, A; Chem Z 1998, V32, P6 HCAPLUS
- (5) Arduengo, A; J Am Chem Soc 1992, V114, P5530 HCAPLUS
- (6) Campion, B; J Chem Soc Chem Commun 1998, P278
- (7) Collman, J; Principles and Applications of Organotransition Metal
Chemistry, 2nd 1987
- (8) Demonceau, A; Macromolecules 1997, V30, P3127 HCAPLUS
- (9) Diaz, E; J Am Chem Soc 1997, V119, P3887
- (10) Fagan, P; J Am Chem Soc 1998, V110, P2981
- (11) Herrmann, W; Angew Chem Int Ed Engl 1996, V35, P1087 HCAPLUS
- (12) Huang, J; J Am Chem Soc 1999, V121, P2674 HCAPLUS
- (13) Huang, J; Organometallics 1999, V18, P2370 HCAPLUS
- (14) Kilday, M; Res Natl Bur Stand (US) 1980, V85, P467 HCAPLUS
- (15) Kingsbury, J; J Am Chem Soc 1999, V121, P791 HCAPLUS
- (16) Lappert, M; J Organomet Chem 1988, V358, P185 HCAPLUS
- (17) Luo, L; Organometallics 1994, V13, P4781 HCAPLUS
- (18) Mohr, B; Organometallics 1996, V15, P4317 HCAPLUS
- (19) Nguyen, S; J Am Chem Soc 1992, V114, P3974 HCAPLUS
- (20) Nguyen, S; J Am Chem Soc 1993, V115, P9858 HCAPLUS
- (21) Nolan, S; Inorg Chem 1986, V25, P4446 HCAPLUS
- (22) Nolan, S; J Organomet Chem 1985, V282, P357 HCAPLUS
- (23) Ojelund, G; Acta Chem Scand 1968, V22, P1691
- (24) Parshall, G; Homogeneous Catalysis 1992
- (25) Perrin, D; Purification of Laboratory Chemicals 1988
- (26) Pignolet, L; Homogeneous Catalysis with Metal Phosphine Complexes 1983

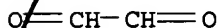
(27) Scholl, M; Tetrahedron Lett 1999, V40, P2247 HCAPLUS
 (28) Schwab, P; Angew Chem Int Ed Engl 1995, V34, P2039 HCAPLUS
 (29) Schwab, P; J Am Chem Soc 1996, V118, P100 HCAPLUS
 (30) Serron, S; Organometallics 1998, V13, P534
 (31) Stumpf, A; J Chem Soc Chem Commun 1995, P1127
 (32) Ulman, M; Organometallics 1998, V17, P2484 HCAPLUS
 (33) Wanzlick, H; Angew Chem Int Ed Engl 1962, V1, P75
 (34) Wu, Z; J Am Chem Soc 1995, V117, P5503 HCAPLUS
 (35) Yang, K; Organometallics 1997, V16, P5234 HCAPLUS
 IT 250285-32-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and neutralization of)
 RN 250285-32-6 HCAPLUS
 CN 1H-Imidazolium, 1,3-bis[2,6-bis(1-methylethyl)phenyl]-, chloride (9CI)
 (CA INDEX NAME)



● Cl⁻

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

IT 107-22-2, Glyoxal
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction with diisopropylaniline)
 RN 107-22-2 HCAPLUS
 CN Ethanedial (9CI) (CA INDEX NAME)



✓ L62 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:798077 HCAPLUS
 DN 132:151738
 ED Entered STN: 19 Dec 1999
 TI Imidazolylidenes, imidazolinylidenes and imidazolidines
 AU Arduengo, Anthony J., III; Krafczyk, Roland; Schmutzler, Reinhard; Craig,
 Hugh A.; Goerlich, Jens R.; Marshall, William J.; Unverzagt, Markus
 CS Institut für Anorganische und Analytische Chemie, der Technischen
 Universität - Carolo Wilhelmina, Braunschweig, D-38106, Germany
 SO Tetrahedron (1999), 55(51), 14523-14534
 CODEN: TETRAB; ISSN: 0040-4020
 PB Elsevier Science Ltd.
 DT Journal
 LA English

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
OS CASREACT 132:151738
AB Starting from **glyoxal** and RNH₂ [R = 2,4,6-Me₃C₆H₂,
2,6-(Me₂CH)₂C₆H₃], the corresponding 1,3-diarylimidazolinium chlorides
were obtained in a 3-step sequence via diimines and ethylenediamine
dihydrochlorides. Subsequent reduction with LiAlH₄ furnished
1,3-diarylimidazolidines, while their deprotonation with KH in THF gave
access to stable carbenes, 1,3-diarylimidazolin-2-ylidenes. Similarly
substituted imidazol-2-ylidenes are described for comparison.
ST **glyoxal** aniline cyclocondensation; imidazolylidene prepn;
imidazolinylidene prepn; imidazolidine prepn
IT Carbenes (methylene derivatives)
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and structure of imidazolylidenes and imidazolinylidenes)
IT 258278-26-1P 258278-31-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure)
IT 244187-81-3P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(crystal structure and chlorination)
IT 250285-32-6P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation)
; PREP (Preparation); RACT (Reactant or reagent)
(crystal structure and reduction)
IT 88-05-1, 2,4,6-Trimethylaniline 107-22-2, **Glyoxal**
3188-13-4, Chloromethyl ethyl ether 24544-04-5, 2,6-Diisopropylaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of imidazolylidenes, imidazolinylidenes, and imidazolidines)
IT 56222-36-7P 74663-75-5P 141556-42-5P 141556-45-8P
173035-10-4P 258278-23-8P 258278-24-9P 258278-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of imidazolylidenes, imidazolinylidenes, and imidazolidines)
IT 173035-11-5P 200730-48-9P 258278-27-2P 258278-28-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of imidazolylidenes, imidazolinylidenes, and imidazolidines)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Alder, R; Angew Chem, Int Ed Engl 1996, V35, P1121 HCAPLUS
(2) Alder, R; Chem Commun (Cambridge) 1997, P1513 HCAPLUS
(3) Alder, R; J Am Chem Soc 1998, V120, P11526 HCAPLUS
(4) Arduengo, A; Angew Chem, Int Ed Engl 1998, V37, P1963 HCAPLUS
(5) Arduengo, A; J Am Chem Soc 1992, V114, P5530 HCAPLUS
(6) Arduengo, A; J Am Chem Soc 1994, V116, P6361 HCAPLUS
(7) Arduengo, A; J Am Chem Soc 1995, V117, P11027 HCAPLUS
(8) Arduengo, A; J Am Chem Soc 1995, V117, P572 HCAPLUS
(9) Arduengo, A; J Am Chem Soc 1997, V119, P12742 HCAPLUS
(10) Arduengo, A; Liebigs Ann 1997, P365 HCAPLUS
(11) Arduengo, A; Organometallics 1998, V17, P3375 HCAPLUS
(12) Arduengo, A; US 5077414 Preparation of 1,3-Disubstituted Imidazolium Salts
1991 HCAPLUS
(13) Arduengo, A; To be published in Acc Chem Res 1999, P32
(14) Arduengo, A; unpublished results
(15) Chen, H; Inorg Chem 1991, V30, P2487 HCAPLUS
(16) Denk, M; Angew Chem, Int Ed Engl 1997, V36, P2607 HCAPLUS
(17) Herrmann, W; Chem-Eur J 1996, V2, P772 HCAPLUS
(18) Hocker, J; Chem Ber 1972, V105, P1651 HCAPLUS
(19) Hocker, J; Justus Liebigs Ann Chem 1971, V751, P145 HCAPLUS
(20) Huang, J; J Am Chem Soc 1999, V121, P2674 HCAPLUS
(21) Huang, J; Organometallics 1999, V18, P2370 HCAPLUS
(22) Jaenicke, L; Liebigs Ann Chem 1959, V624, P120 HCAPLUS

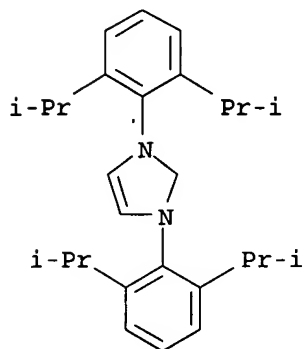
- (23) Jafarpour, L; Organometallics 1999, V18, P3760 HCAPLUS
- (24) Keller, E; SCHAKAL
- (25) Kuhn, N; Synthesis 1993, V1993, P561
- (26) Nishiyama, T; J Heterocycl Chem 1988, V25, P1773 HCAPLUS
- (27) Perrin, D; Purification of Laboratory Chemicals; 2nd ed 1985
- (28) Taton, T; Angew Chem, Int Ed Engl 1996, V35, P1011 HCAPLUS
- (29) Wanzlick, H; Angew Chem 1960, V72, P494 HCAPLUS
- (30) Wanzlick, H; Angew Chem 1962, V74, P128
- (31) Wanzlick, H; Chem Ber 1953, V86, P1463 HCAPLUS
- (32) Wanzlick, H; Chem Ber 1961, V74, P2389
- (33) Wanzlick, H; Chem Ber 1963, V96, P1208 HCAPLUS
- (34) Zettlitzer, M; Chem Ber 1986, V119, P1868 HCAPLUS
- (35) Zhang, C; J Org Chem 1999, V64, P3804 HCAPLUS

IT 250285-32-6P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation)
; PREP (Preparation); RACT (Reactant or reagent)
(crystal structure and reduction).

RN 250285-32-6 HCAPLUS

CN 1H-Imidazolium, 1,3-bis[2,6-bis(1-methylethyl)phenyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

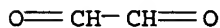
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

IT 107-22-2, Glyoxal

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of imidazolyliidenes, imidazolinylidenes, and imidazolidines)

RN 107-22-2 HCAPLUS

CN Ethanedial (9CI) (CA INDEX NAME)

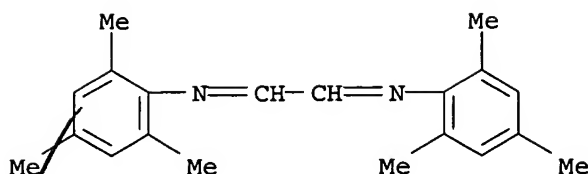


IT 56222-36-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of imidazolyliidenes, imidazolinylidenes, and imidazolidines)

RN 56222-36-7 HCAPLUS

CN Benzenamine, N,N'-1,2-ethanediylidenebis[2,4,6-trimethyl- (9CI) (CA INDEX
NAME)



L62 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1999:643360 HCAPLUS
 DN 132:49760
 ED Entered STN: 11 Oct 1999
 TI Efficient Cross-Coupling of Aryl Chlorides with Aryl Grignard Reagents
 (Kumada Reaction) Mediated by a Palladium/Imidazolium Chloride System
 AU Huang, Jinkun; Nolan, Steven P.
 CS Department of Chemistry, University of New Orleans, New Orleans, LA,
 70148, USA
 SO Journal of the American Chemical Society (1999), 121(42),
 9889-9890
 CODEN: JACSAT; ISSN: 0002-7863
 PB American Chemical Society
 DT Journal
 LA English
 CC 25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 OS CASREACT 132:49760
 AB A general methodol. for the Kumada reaction was presented. In the
 presence of tris[μ-[(1,2-η:4,5-η)-(1E,4E)-1,5-diphenyl-1,4-
 pentadien-3-one]]dipalladium or palladium diacetate and an imidazolium
 chloride, aryl chlorides, aryl bromides or aryl iodides underwent a
 coupling reaction to give biphenyl derivs. Suitable imidazolium compds.
 were 1,3-bis(2,4,6-trimethylphenyl)-1H-imidazolium chloride and
 1,3-bis[2,6-bis(1-methylethyl)phenyl]-1H-imidazolium chloride.
 ST crosscoupling aryl chloride Grignard reagent Kumada; biphenyl
 phenylnaphthalene prepn
 IT Cross-coupling reaction
 (Kumada reaction; cross-coupling of aryl chlorides with aryl Grignard
 reagents (Kumada reaction) mediated by palladium and imidazolium
 chloride)
 IT Aryl halides
 Aryl halides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aryl chlorides; cross-coupling of aryl chlorides with aryl Grignard
 reagents (Kumada reaction) mediated by palladium and imidazolium
 chloride)
 IT Aryl halides
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aryl iodides; cross-coupling of aryl chlorides with aryl Grignard
 reagents (Kumada reaction) mediated by palladium and imidazolium
 chloride)
 IT Chlorides, reactions
 Chlorides, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aryl; cross-coupling of aryl chlorides with aryl Grignard reagents
 (Kumada reaction) mediated by palladium and imidazolium chloride)
 IT Cross-coupling reaction catalysts
 (cross-coupling of aryl chlorides with aryl Grignard reagents (Kumada
 reaction) mediated by palladium and imidazolium chloride)
 IT Aryl bromides
 Grignard reagents
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cross-coupling of aryl chlorides with aryl Grignard reagents (Kumada

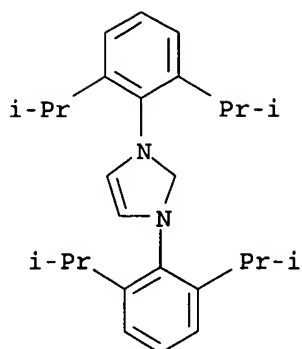
- reaction) mediated by palladium and imidazolium chloride)
- IT 3375-31-3, Palladium diacetate 51364-51-3, Tris[μ -(1,2- η :4,5- η)-(1E,4E)-1,5-diphenyl-1,4-pentadien-3-one]]dipalladium
141556-45-8, 1,3-Bis(2,4,6-trimethylphenyl)-1H-imidazolium chloride
RL: CAT (Catalyst use); USES (Uses)
(cross-coupling of aryl chlorides with aryl Grignard reagents mediated by palladium and imidazolium chloride)
- IT 250285-32-6P, 1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1H-imidazolium chloride
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(cross-coupling of aryl chlorides with aryl Grignard reagents mediated by palladium and imidazolium chloride)
- IT 95-72-7, 1-Chloro-2,5-dimethylbenzene 100-58-3, Phenylmagnesium bromide
106-38-7, 1-Bromo-4-methylbenzene 106-43-4, 1-Chloro-4-methylbenzene
106-48-9, 4-Chlorophenol 107-22-2, Glyoxal 446-53-7,
(2-Fluorophenyl)magnesium bromide 540-38-5, 4-Iodophenol 619-42-1
623-12-1, 1-Chloro-4-methoxybenzene 2633-66-1, (2,4,6-Trimethylphenyl)magnesium bromide 4294-57-9, (4-Methylphenyl)magnesium bromide 5111-65-9, 2-Bromo-6-methoxynaphthalene 6781-98-2,
1-Chloro-2,6-dimethylbenzene 24544-04-5, 2,6-Diisopropylaniline 28987-79-3, (3-Methylphenyl)magnesium bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(cross-coupling of aryl chlorides with aryl Grignard reagents mediated by palladium and imidazolium chloride)
- IT 74663-75-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cross-coupling of aryl chlorides with aryl Grignard reagents mediated by palladium and imidazolium chloride)
- IT 92-69-3P, [1,1'-Biphenyl]-4-ol 613-37-6P, 4-Methoxy-1,1'-biphenyl
644-08-6P, 4-Methyl-1,1'-biphenyl 720-75-2P, [1,1'-Biphenyl]-4-carboxylic acid, methyl ester 3976-34-9P, 2,6-Dimethyl-1,1'-biphenyl
7372-85-2P, 2,5-Dimethyl-1,1'-biphenyl 17171-17-4P 39502-90-4P,
4'-Methoxy-2,4,6-trimethyl-1,1'-biphenyl 53040-92-9P,
4-Methoxy-4'-methyl-1,1'-biphenyl 59115-43-4P, 2-Methoxy-6-phenylnaphthalene 72093-47-1P, 2-Fluoro-4'-methoxy-1,1'-biphenyl
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RE.CNT 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Anon; Chem Eng News July 13 71 1998
- (2) Anon; Chem Eng News June 1 1998
- (3) Anon; Homogeneous Catalysis with Metal Phosphine Complexes
- (4) Arduengo, A; Chem Ztg 1998, V32, P6 HCAPLUS
- (5) Arduengo, A; J Am Chem Soc 1992, V116, P4391
- (6) Arduengo, A; J Am Chem Soc 1992, V114, P5530 HCAPLUS
- (7) Barba, I; Tetrahedron 1990, V46, P7813 HCAPLUS
- (8) Bei, X; Tetrahedron Lett 1999, V40, P1237 HCAPLUS
- (9) Bei, X; Tetrahedron Lett 1999, V40, P3855 HCAPLUS
- (10) Bell, H; Aust J Chem 1979, V32, P1531 HCAPLUS
- (11) Bourelle-Warhnier, F; J Org Chem 1980, V45, P428
- (12) Busacca, C; Tetrahedron Lett 1999, V40, P3101 HCAPLUS
- (13) Collman, J; Principles and Applications of Organotransition Metal Chemistry 1987
- (14) Cornils, B; Applied Homogeneous Catalysis with Organometallic Compounds 1996
- (15) Corriu, R; Chem Soc, Chem Commun 1972, P144 HCAPLUS
- (16) Farina, V; J Org Chem 1993, V58, P5434 HCAPLUS
- (17) Hamann, B; J Am Chem Soc 1998, V120, P7369 HCAPLUS
- (18) Hayashi, T; J Am Chem Soc 1982, V104, P180 HCAPLUS
- (19) Hayashi, T; J Am Chem Soc 1984, V106, P158 HCAPLUS
- (20) Heck, R; Palladium Reagents in Organic Syntheses 1985

- (21) Herrmann, W; Angew Chem, Int Ed Engl 1995, V34, P2371 HCAPLUS
(22) Herrmann, W; Angew Chem, Int Ed Engl 1996, V35, P2805 HCAPLUS
(23) Herrmann, W; Angew Chem, Int Ed Engl 1997, V36, P2163
(24) Herrmann, W; Chem Eur J 1996, V2, P772 HCAPLUS
(25) Herrmann, W; J Organomet Chem 1998, V557, P93 HCAPLUS
(26) Huang, J; J Am Chem Soc 1999, V121, P2674 HCAPLUS
(27) Huang, J; Manuscript submitted for publication
(28) Huang, J; Organometallics 1999, V18, P2370 HCAPLUS
(29) Indolese, A; Tetrahedron Lett 1997, V38, P3513 HCAPLUS
(30) Jendralla, H; Synthesis 1990, P827 HCAPLUS
(31) Kamikawa, T; Synlett 1997, P163 HCAPLUS
(32) Kang, S; J Org Chem 1996, V61, P4720 HCAPLUS
(33) Kumada, M; Pure Appl Chem 1980, V52, P669 HCAPLUS
(34) Littke, A; Int Ed Engl 1998, V37, P3387 HCAPLUS
(35) Littke, A; J Org Chem 1999, V64, P10 HCAPLUS
(36) Lourak, M; J Org Chem 1989, V54, P4844 HCAPLUS
(37) McGuinness, D; J Organomet Chem 1998, V165, P16
(38) Miller, J; Tetrahedron Lett 1998, V39, P7275 HCAPLUS
(39) Minato, A; Tetrahedron Lett 1981, V22, P5319 HCAPLUS
(40) Miyaura, N; Chem Rev 1995, V95, P2457 HCAPLUS
(41) Old, D; J Am Chem Soc 1998, V120, P9722 HCAPLUS
(42) Parshall, G; Homogeneous Catalysis 1992
(43) Rao, M; Synthesis 1987, P231
(44) Reetz, M; Angew Chem Int Ed Engl 1998, V37, P481 HCAPLUS
(45) Regitz, M; Angew Chem, Int Ed Engl 1996, V35, P725 HCAPLUS
(46) Saito, S; J Org Chem 1997, V62, P8024 HCAPLUS
(47) Saito, S; Tetrahedron Lett 1996, V37, P2993 HCAPLUS
(48) Schoervarrs, A; J Org Chem 1997, V62, P4943
(49) Scholl, M; Tetrahedron Lett 1999, V40, P2247 HCAPLUS
(50) Sekiya, A; J Organomet 1976, V118, P349 HCAPLUS
(51) Shishido, K; J Chem Soc Perkin Trans 1990, V1, P469
(52) Sofia, A; J Org Chem 1999, V64, P1745
(53) Stanforth, S; Tetrahedron 1998, V54, P263 HCAPLUS
(54) Tamao, K; Bull Chem Soc Jpn 1976, V49, P1958 HCAPLUS
(55) Tamao, K; J Am Chem Soc 1972, V94, P4374 HCAPLUS
(56) Tamao, K; J Am Chem Soc 1972, V94, P9268 HCAPLUS
(57) Trost, B; Comprehensive Organometallic Chemistry 1982, V8, P799
(58) Tsuji, J; Palladium Reagents and Catalysts 1995
(59) Tsuji, J; Synthesis 1990, P739 HCAPLUS
(60) Voges, M; Organometallics 1999, V18, P529 HCAPLUS
(61) Weskamp, T; Angew Chem, Int Ed Engl 1998, V37, P2490 HCAPLUS
(62) Widdowson, D; Tetrahedron 1986, V42, P2111 HCAPLUS
(63) Yamamura, M; J Organomet Chem 1975, V91, P339 HCAPLUS
(64) Zhang, C; J Org Chem, in press 1999
- IT 250285-32-6P, 1,3-Bis[2,6-bis(1-methylethyl)phenyl]-1H-imidazolium chloride
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(cross-coupling of aryl chlorides with aryl Grignard reagents mediated by palladium and imidazolium chloride)
- RN 250285-32-6 HCAPLUS
CN 1H-Imidazolium, 1,3-bis[2,6-bis(1-methylethyl)phenyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

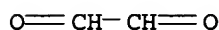
IT 107-22-2, Glyoxal

RL: RCT (Reactant); RACT (Reactant or reagent)

(cross-coupling of aryl chlorides with aryl Grignard reagents mediated by palladium and imidazolium chloride)

RN 107-22-2 HCAPLUS

CN Ethanedial (9CI) (CA INDEX NAME)



=> => fil casreact

FILE 'CASREACT' ENTERED AT 15:53:29 ON 24 MAR 2005

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 20 Mar 2005 VOL 142 ISS 12

```
*****
*
*      CASREACT now has more than 8 million reactions
*
*****
```

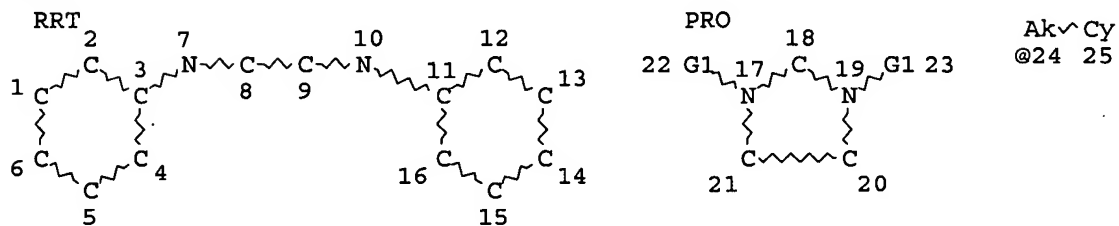
Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d sta que

```
L20      1 SEA FILE=REGISTRY ABB=ON  PLU=ON  PARAFORMALDEHYDE/CN
L21      1 SEA FILE=REGISTRY ABB=ON  PLU=ON  "HYDROCHLORIC ACID"/CN
L22      1 SEA FILE=REGISTRY ABB=ON  PLU=ON  14874-70-5
```

L23 3 SEA FILE=REGISTRY ABB=ON PLU=ON F6P/MF
 L27 5 SEA FILE=REGISTRY ABB=ON PLU=ON (METHANOL OR ETHYL ACETATE
 OR ETHANOL OR TETRAHYDROFURAN OR TOLUENE)/CN
 L67 STR

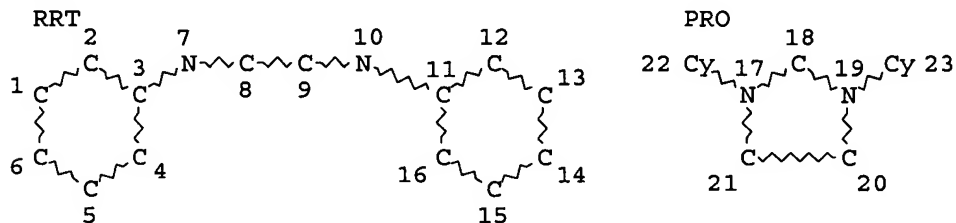


VAR G1=AK/CY/24
 NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE

L69 98 SEA FILE=CASREACT SSS FUL L67 (361 REACTIONS)
 L70 23 SEA FILE=CASREACT ABB=ON PLU=ON L69 AND (L20 OR L21 OR L22
 OR L23)
 L71 21 SEA FILE=CASREACT ABB=ON PLU=ON L70 AND L27
 L72 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

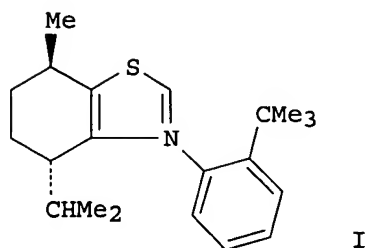
L73 96 SEA FILE=CASREACT SUB=L69 SSS FUL L72 (348 REACTIONS)
 L74 23 SEA FILE=CASREACT ABB=ON PLU=ON L73 AND L70
 L75 6 SEA FILE=CASREACT ABB=ON PLU=ON L74 AND (IMIDAZOL? OR
 DIARYLIMID?)/TI
 L76 4 SEA FILE=CASREACT ABB=ON PLU=ON L75 NOT (OXALA? OR OXALIC?)/T
 I
 L77 4 SEA FILE=CASREACT ABB=ON PLU=ON L76 AND (L70 OR L71 OR L74)

=> d bib abs fhit retable tot

L77 ANSWER 1 OF 4 CASREACT COPYRIGHT 2005 ACS on STN
 AN 141:140358 CASREACT
 TI Preparation of axially chiral N,N'-diarylimidazolium and

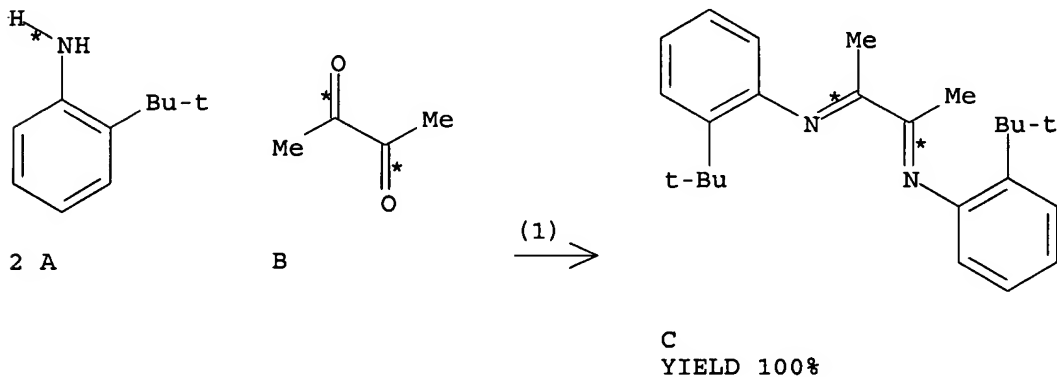
N-arylthiazolium salts and evaluation of their catalytic potential in the benzoin and in the intramolecular Stetter reactions

AU Pesch, Jens; Harms, Klaus; Bach, Thorsten
 CS Lehrstuhl fuer Organische Chemie I, Technische Universitaet Muenchen, Garching, 85747, Germany
 SO European Journal of Organic Chemistry (2004), (9), 2025-2035
 CODEN: EJOCFK; ISSN: 1434-193X
 PB Wiley-VCH Verlag GmbH & Co. KGaA
 DT Journal
 LA English
 GI



AB N-Aryl-substituted imidazoles were prepared which contain a stereogenic axis and which can occur as atropisomers. The di(2-isopropylphenyl)imidazolium salts could be obtained from 2-isopropylaniline and diacetyl in three steps (19% yield) whereas the synthesis of their tert-Bu analogs failed. The meso-isomer prevailed (dr = 90/10). Chiral thiazolium salts were prepared in two steps from 2-tert-butylaniline. The enantiomerically pure thiazolium salt I was obtained from α -bromomenthone and 2-tert-butylaniline (27% overall yield). In contrast to the imidazolium salts, the thiazolium salts proved to be suitable catalysts in the benzoin condensation of benzaldehyde and in the intramol. Stetter reaction of 2-OCHC6H4OCH2CH:CHCO2Me. The best results obtained with catalyst I (20 mol %) were 85% (R)-PhCOCHPhOH (40% ee) and 75% Me (R)-4-oxochroman-3-acetate. The stereogenic axis of I is not configurationally stable in the catalytically active carbene intermediate. The catalyst is recovered as a mixture of diastereomeric atropisomers in a ratio of 70:30 to 75:25.

RX(1) OF 30 2 A + B ==> C



RX(1) RCT A 6310-21-0, B 431-03-8

PRO C 181707-42-6
 CAT 64-18-6 HCO2H
 SOL 64-17-5 EtOH

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Arduengo, A	1999	32	913	Acc Chem Res	CAPLUS
Arduengo, A	1998	110	2062	Angew Chem	
Arduengo, A	1998	37	1963	Angew Chem Int Ed	CAPLUS
Bach, T	1999	40	9003	Tetrahedron Lett	CAPLUS
Bourissou, D	2000	100	39	Chem Rev	CAPLUS
Breslow, R	1958	80	3719	J Am Chem Soc	CAPLUS
Breslow, R	1959	81	3080	J Am Chem Soc	CAPLUS
Breslow, R	1996	37	8241	Tetrahedron Lett	CAPLUS
CCDC				www.ccdc.cam.ac.uk/c	
CCDC				www.ccdc.cam.ac.uk/c	
CCDC				www.ccdc.cam.ac.uk/c	
CCDC				www.ccdc.cam.ac.uk/c	
CCDC				www.ccdc.cam.ac.uk/c	
Ciganek, E	1995		1311	Synthesis	CAPLUS
Djafri, A	1985		273	J Chem Soc, Perkin T	CAPLUS
Djafri, A	1996	6	123	J Soc, Alger Chim	CAPLUS
Dvorak, C	1998	39	2925	Tetrahedron Lett	CAPLUS
Enders, D	2002	114	1822	Angew Chem	
Enders, D	2002	41	1743	Angew Chem Int Ed	CAPLUS
Enders, D	1999	3	1093	Comprehensive Asymme	CAPLUS
Enders, D	1996	79	1217	Helv Chim Acta	CAPLUS
Enders, D	1996	79	1899	Helv Chim Acta	CAPLUS
Enders, D	2003		1292	Synthesis	CAPLUS
Gallo, R	1988	43	173	Adv Heterocycl Chem	CAPLUS
Gerhard, A	1997	38	3615	Tetrahedron Lett	CAPLUS
Hassner, A	1991	1	541	Comprehensive Organi	
Herrmann, W	1997	109	2256	Angew Chem	
Herrmann, W	2002	114	1342	Angew Chem	
Herrmann, W	2002	41	1290	Angew Chem Int Ed	CAPLUS
Herrmann, W	1997	36	2162	Angew Chem Int Ed En	CAPLUS
Hirtopceanu, A	2000		1081	Eur J Org Chem	CAPLUS
Hirtopceanu, A	2000	53	1669	Heterocycles	CAPLUS
Ide, W	1948	4	269	Org React	CAPLUS
Kerr, M	2002	124	10298	J Am Chem Soc	CAPLUS
Kerr, M	2003		1934	Synlett	CAPLUS
Knight, R	1997	38	3611	Tetrahedron Lett	CAPLUS
Leeper, F	1995		861	J Chem Soc, Perkin T	CAPLUS
Leeper, F	1998		1891	J Chem Soc, Perkin T	
Liebscher, J	1994	E8b	192	Houben-Weyl, 4th ed	
Marti, J	1993	34	521	Tetrahedron Lett	CAPLUS
Pesch, J	2000			Diploma Thesis, Univ	
Peters, K	1998	213	503	Z Kristallogr	CAPLUS
Pohl, M	2002	8	5288	Chem Eur J	CAPLUS
Regitz, M	1996	108	791	Angew Chem	
Regitz, M	1997	35	724	Angew Chem Int Ed En	
Roussel, C	1997	761	129	J Chromatogr A	CAPLUS
Roussel, C	1988	53	5076	J Org Chem	CAPLUS
Roussel, C	1988	12	947	New J Chem	CAPLUS
Schönherr, H	1970	731	176	Justus Liebigs Ann C	
Seiders, T	2001	3	3225	Org Lett	CAPLUS
Sheehan, J	1966	88	3666	J Am Chem Soc	CAPLUS
Sheehan, J	1974	39	1196	J Org Chem	CAPLUS
Stetter, H	1973	85	89	Angew Chem	CAPLUS
Stetter, H	1974	86	589	Angew Chem	CAPLUS
Stetter, H	1976	88	695	Angew Chem	CAPLUS
Stetter, H	1973	12	81	Angew Chem Int Ed En	

Stetter, H	1974	13	539	Angew Chem Int Ed En	
Stetter, H	1976	15	639	Angew Chem Int Ed En	
Stetter, H	1991	40	407	Org React	CAPLUS
Still, W	1978	43	2923	J Org Chem	CAPLUS
Tagaki, W	1980	53	478	Bull Chem Soc Jpn	CAPLUS
Teles, J	1996	79	61	Helv Chim Acta	CAPLUS
Tempel, D	2000	122	6686	J Am Chem Soc	CAPLUS
Ukai, T	1943	63	112	J Pharm Soc, Jpn	
Uscumlic, G	1994		1799	J Chem Soc, Perkin T	CAPLUS
Wohler, F	1832	3	249	Ann Pharm	
Wolf, C	1995		781	Liebigs Ann	CAPLUS
Zhao, C	1988	46	784	Huaxue Xuebao	CAPLUS

L77 ANSWER 2 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

AN 133:362823 CASREACT

TI A sterically demanding nucleophilic carbene: 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene. Thermochemistry and catalytic application in olefin metathesis

AU Jafarpour, L.; Stevens, E. D.; Nolan, S. P.

CS Department of Chemistry, University of New Orleans, New Orleans, LA, 70148, USA

SO Journal of Organometallic Chemistry (2000), 606(1), 49-54
CODEN: JORCAI; ISSN: 0022-328X

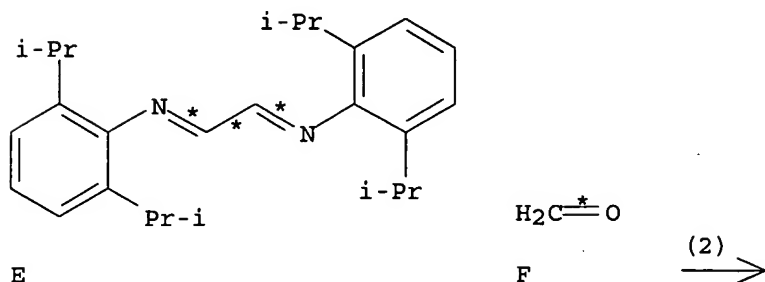
PB Elsevier Science S.A.

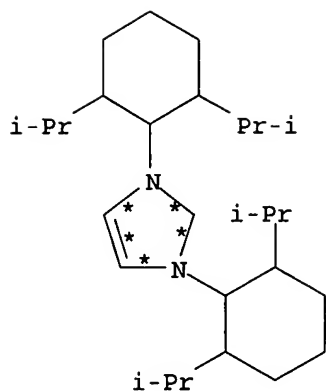
DT Journal

LA English

AB The sterically demanding nucleophilic carbene ligand 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene (IPr, 4) has been synthesized. The reaction of [Cp*RuCl]₄ (5; Cp* = η⁵-C₅Me₅) with this ligand affords a coordinatively unsatd. Cp*Ru(IPr)Cl (6) complex. Solution calorimetric results in this system provide information concerning the electron donor properties of the carbene ligand. Steric parameters associated with this ligand are determined from the x-ray crystal structure study. The carbene ligand reacts with RuCl₂(C(H)Ph)(PCy₃)₂ to yield a mixed carbene-phosphine ruthenium complex RuCl₂(C(H)Ph)(IPr)(PCy₃) (9). A single-crystal x-ray diffraction study has been performed on 9. The thermal stability of 9 has been studied at 60° and its catalytic activity has been evaluated for the ring closing metathesis of di-Et diallylmalonate.

RX(2) OF 15 ...E + F ==> G...





● Cl⁻

G
YIELD 47%

RX(2) RCT E 74663-75-5, F 50-00-0

STAGE(1)

SOL 108-88-3 PhMe

STAGE(2)

RGT H 7647-01-0 HCl

SOL 123-91-1 Dioxane

PRO G 250285-32-6

NTE PARAFORMALDEHYDE USED

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Ackermann, L	1999	40	4787	Tetrahedron Lett	CAPLUS
Anon				private communicatio	
Arduengo, A	1991			US 5077414	CAPLUS
Arduengo, A	1998	32	6	Chem Z	CAPLUS
Arduengo, A	1992	114	5530	J Am Chem Soc	CAPLUS
Campion, B	1998		278	J Chem Soc Chem Comm	
Collman, J	1987			Principles and Appli	
Demonceau, A	1997	30	3127	Macromolecules	CAPLUS
Diaz, E	1997	119	3887	J Am Chem Soc	
Fagan, P	1998	110	2981	J Am Chem Soc	
Herrmann, W	1996	35	1087	Angew Chem Int Ed En	CAPLUS
Huang, J	1999	121	2674	J Am Chem Soc	CAPLUS
Huang, J	1999	18	2370	Organometallics	CAPLUS
Kilday, M	1980	85	467	Res Natl Bur Stand (CAPLUS
Kingsbury, J	1999	121	791	J Am Chem Soc	CAPLUS
Lappert, M	1988	358	185	J Organomet Chem	CAPLUS
Luo, L	1994	13	4781	Organometallics	CAPLUS
Mohr, B	1996	15	4317	Organometallics	CAPLUS
Nguyen, S	1992	114	3974	J Am Chem Soc	CAPLUS
Nguyen, S	1993	115	9858	J Am Chem Soc	CAPLUS
Nolan, S	1986	25	4446	Inorg Chem	CAPLUS
Nolan, S	1985	282	357	J Organomet Chem	CAPLUS
Ojelund, G	1968	22	1691	Acta Chem Scand	
Parshall, G	1992			Homogeneous Catalysi	

Perrin, D	1988			Purification of Labo	
Pignolet, L	1983			Homogeneous Catalysi	
Scholl, M	1999	40	2247	Tetrahedron Lett	CAPLUS
Schwab, P	1995	34	2039	Angew Chem Int Ed En	CAPLUS
Schwab, P	1996	118	100	J Am Chem Soc	CAPLUS
Serron, S	1998	13	534	Organometallics	
Stumpf, A	1995		1127	J Chem Soc Chem Comm	
Ulman, M	1998	17	2484	Organometallics	CAPLUS
Wanzlick, H	1962	1	75	Angew Chem Int Ed En	
Wu, Z	1995	117	5503	J Am Chem Soc	CAPLUS
Yang, K	1997	16	5234	Organometallics	CAPLUS

L77 ANSWER 3 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

AN 132:151738 CASREACT

TI **Imidazolylidenes, imidazolinylienes and imidazolidines**

AU Arduengo, Anthony J., III; Krafczyk, Roland; Schmutzler, Reinhard; Craig, Hugh A.; Goerlich, Jens R.; Marshall, William J.; Unverzagt, Markus

CS Institut fur Anorganische und Analytische Chemie, der Technischen Universitat - Carolo Wilhelmina, Braunschweig, D-38106, Germany

SO Tetrahedron (1999), 55(51), 14523-14534

CODEN: TETRAB; ISSN: 0040-4020

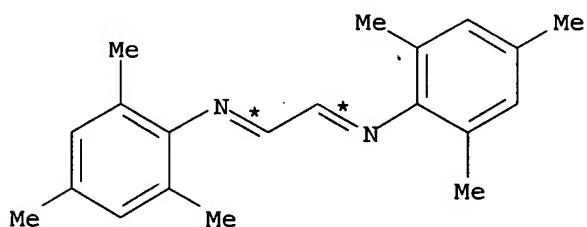
PB Elsevier Science Ltd.

DT Journal

LA English

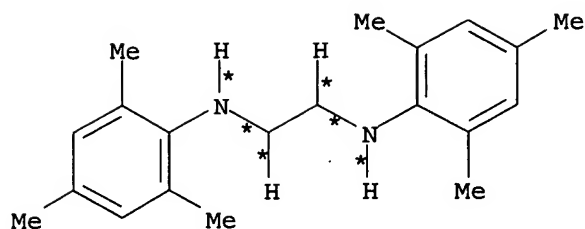
AB Starting from glyoxal and RNH₂ [R = 2,4,6-Me₃C₆H₂, 2,6-(Me₂CH)₂C₆H₃], the corresponding 1,3-diarylimidazolium chlorides were obtained in a 3-step sequence via diimines and ethylenediamine dihydrochlorides. Subsequent reduction with LiAlH₄ furnished 1,3-diarylimidazolidines, while their deprotonation with KH in THF gave access to stable carbenes, 1,3-diarylimidazol-2-ylidenes. Similarly substituted imidazol-2-ylidenes are described for comparison.

RX(1) OF 14 A ==> B



A





● 2 HCl

B
YIELD 85%

RX(1) RCT A 56222-36-7

STAGE(1)

RGT C 16940-66-2 NaBH₄

SOL 109-99-9 THF

STAGE(2)

RGT D 7647-01-0 HCl

SOL 7732-18-5 Water, 76-05-1 F3CCO₂H

PRO B 258278-23-8

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
=====	=====	=====	=====	=====	=====
Alder, R	1996	35	1121	Angew Chem, Int Ed E	CAPLUS
Alder, R	1997		1513	Chem Commun (Cambrid	CAPLUS
Alder, R	1998	120	11526	J Am Chem Soc	CAPLUS
Arduengo, A	1998	37	1963	Angew Chem, Int Ed E	CAPLUS
Arduengo, A	1992	114	5530	J Am Chem Soc	CAPLUS
Arduengo, A	1994	116	6361	J Am Chem Soc	CAPLUS
Arduengo, A	1995	117	11027	J Am Chem Soc	CAPLUS
Arduengo, A	1995	117	572	J Am Chem Soc	CAPLUS
Arduengo, A	1997	119	12742	J Am Chem Soc	CAPLUS
Arduengo, A	1997		365	Liebigs Ann	CAPLUS
Arduengo, A	1998	17	3375	Organometal	CAPLUS
Arduengo, A	1991			US 5077414	CAPLUS
Arduengo, A	1999		32	To be published in A	
Arduengo, A				unpublished results	
Chen, H	1991	30	2487	Inorg Chem	CAPLUS
Denk, M	1997	36	2607	Angew Chem, Int Ed E	CAPLUS
Herrmann, W	1996	2	772	Chem-Eur J	CAPLUS
Hocker, J	1972	105	1651	Chem Ber	CAPLUS
Hocker, J	1971	751	145	Justus Liebigs Ann C	CAPLUS
Huang, J	1999	121	2674	J Am Chem Soc	CAPLUS
Huang, J	1999	18	2370	Organometallics	CAPLUS
Jaenicke, L	1959	624	120	Liebigs Ann Chem	CAPLUS
Jafarpour, L	1999	18	3760	Organometallics	CAPLUS
Keller, E				SCHAKAL	
Kuhn, N	1993	1993	561	Synthesis	
Nishiyama, T	1988	25	1773	J Heterocycl Chem	CAPLUS
Perrin, D	1985			Purification of Labo	
Taton, T	1996	35	1011	Angew Chem, Int Ed E	CAPLUS
Wanzlick, H	1960	72	494	Angew Chem	CAPLUS
Wanzlick, H	1962	74	128	Angew Chem	

Wanzlick, H	1953	86	1463	Chem Ber	CAPLUS
Wanzlick, H	1961	74	2389	Chem Ber	
Wanzlick, H	1963	96	1208	Chem Ber	CAPLUS
Zettlitz, M	1986	119	1868	Chem Ber	CAPLUS
Zhang, C	1999	64	3804	J Org Chem	CAPLUS

L77 ANSWER 4 OF 4 CASREACT COPYRIGHT 2005 ACS on STN

AN 132:49760 CASREACT

TI Efficient Cross-Coupling of Aryl Chlorides with Aryl Grignard Reagents
(Kumada Reaction) Mediated by a Palladium/Imidazolium Chloride
System

AU Huang, Jinkun; Nolan, Steven P.

CS Department of Chemistry, University of New Orleans, New Orleans, LA,
70148, USA

SO Journal of the American Chemical Society (1999), 121(42), 9889-9890
CODEN: JACSAT; ISSN: 0002-7863

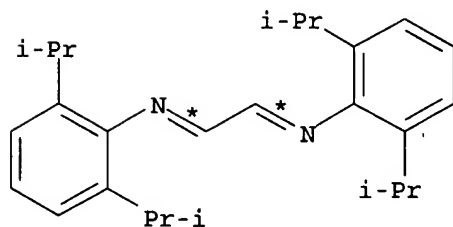
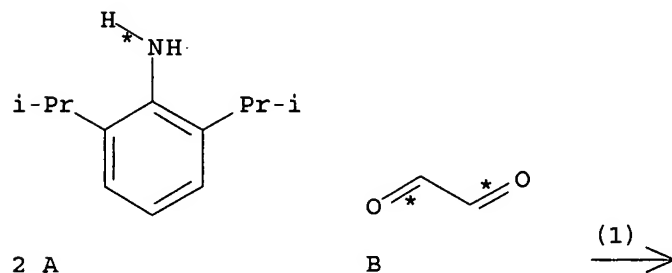
PB American Chemical Society

DT Journal

LA English

AB A general methodol. for the Kumada reaction was presented. In the
presence of tris[μ-[(1,2-η:4,5-η)-(1E,4E)-1,5-diphenyl-1,4-
pentadien-3-one]]dipalladium or palladium diacetate and an imidazolium
chloride, aryl chlorides, aryl bromides or aryl iodides underwent a
coupling reaction to give biphenyl derivs. Suitable imidazolium compds.
were 1,3-bis(2,4,6-trimethylphenyl)-1H-imidazolium chloride and
1,3-bis[2,6-bis(1-methylethyl)phenyl]-1H-imidazolium chloride.

RX(1) OF 16 2 A + B ==> C...



C
YIELD 78%

RX(1) RCT A 24544-04-5, B 107-22-2
PRO C 74663-75-5
CAT 64-18-6 HCO2H

SOL 7732-18-5 Water, 64-17-5 EtOH

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
=====	=====	=====	=====	=====	=====
Anon	1998			Chem Eng News July 1	
Anon	1998			Chem Eng News June 1	
Anon				Homogeneous Catalysi	
Arduengo, A	1998	32	6	Chem Ztg	CAPLUS
Arduengo, A	1992	116	4391	J Am Chem Soc	
Arduengo, A	1992	114	5530	J Am Chem Soc	CAPLUS
Barba, I	1990	46	7813	Tetrahedron	CAPLUS
Bei, X	1999	40	1237	Tetrahedron Lett	CAPLUS
Bei, X	1999	40	3855	Tetrahedron Lett	CAPLUS
Bell, H	1979	32	1531	Aust J Chem	CAPLUS
Bourelle-Warhnier, F	1980	45	428	J Org Chem	
Busacca, C	1999	40	3101	Tetrahedron Lett	CAPLUS
Collman, J	1987			Principles and Appli	
Cornils, B	1996			Applied Homogeneous	
Corriu, R	1972		144	Chem Soc, Chem Commu	CAPLUS
Farina, V	1993	58	5434	J Org Chem	CAPLUS
Hamann, B	1998	120	7369	J Am Chem Soc	CAPLUS
Hayashi, T	1982	104	180	J Am Chem Soc	CAPLUS
Hayashi, T	1984	106	158	J Am Chem Soc	CAPLUS
Heck, R	1985			Palladium Reagents i	
Herrmann, W	1995	34	2371	Angew Chem, Int Ed E	CAPLUS
Herrmann, W	1996	35	2805	Angew Chem, Int Ed E	CAPLUS
Herrmann, W	1997	36	2163	Angew Chem, Int Ed E	
Herrmann, W	1996	2	772	Chem Eur J	CAPLUS
Herrmann, W	1998	557	93	J Organomet Chem	CAPLUS
Huang, J	1999	121	2674	J Am Chem Soc	CAPLUS
Huang, J				Manuscript submitted	
Huang, J	1999	18	2370	Organometallics	CAPLUS
Indolese, A	1997	38	3513	Tetrahedron Lett	CAPLUS
Jendralla, H	1990		827	Synthesis	CAPLUS
Kamikawa, T	1997		163	Synlett	CAPLUS
Kang, S	1996	61	4720	J Org Chem	CAPLUS
Kumada, M	1980	52	669	Pure Appl Chem	CAPLUS
Littke, A	1998	37	3387	Int Ed Engl	CAPLUS
Littke, A	1999	64	10	J Org Chem	CAPLUS
Lourak, M	1989	54	4844	J Org Chem	CAPLUS
McGuinness, D	1998	165	16	J Organomet Chem	
Miller, J	1998	39	7275	Tetrahedron Lett	CAPLUS
Minato, A	1981	22	5319	Tetrahedron Lett	CAPLUS
Miyaura, N	1995	95	2457	Chem Rev	CAPLUS
Old, D	1998	120	9722	J Am Chem Soc	CAPLUS
Parshall, G	1992			Homogeneous Catalysi	
Rao, M	1987		231	Synthesis	
Reetz, M	1998	37	481	Angew Chem Int Ed En	CAPLUS
Regitz, M	1996	35	725	Angew Chem, Int Ed E	CAPLUS
Saito, S	1997	62	8024	J Org Chem	CAPLUS
Saito, S	1996	37	2993	Tetrahedron Lett	CAPLUS
Schoervarrs, A	1997	62	4943	J Org Chem	
Scholl, M	1999	40	2247	Tetrahedron Lett	CAPLUS
Sekiya, A	1976	118	349	J Organomet	CAPLUS
Shishido, K	1990	1	469	J Chem Soc Perkin Tr	
Sofia, A	1999	64	1745	J Org Chem	
Stanforth, S	1998	54	263	Tetrahedron	CAPLUS
Tamao, K	1976	49	1958	Bull Chem Soc Jpn	CAPLUS
Tamao, K	1972	94	4374	J Am Chem Soc	CAPLUS
Tamao, K	1972	94	9268	J Am Chem Soc	CAPLUS
Trost, B	1982	8	799	Comprehensive Organo	
Tsuji, J	1995			Palladium Reagents a	

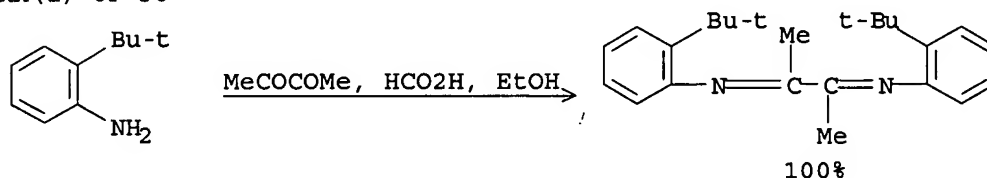
Tsuiji, J	1990		739	Synthesis	CAPLUS
Voges, M	1999	18	529	Organometallics	CAPLUS
Weskamp, T	1998	37	2490	Angew Chem, Int Ed E	CAPLUS
Widdowson, D	1986	42	2111	Tetrahedron	CAPLUS
Yamamura, M	1975	91	C39	J Organomet Chem	CAPLUS
Zhang, C	1999			J Org Chem, in press	

=> d scan

L77 4 ANSWERS CASREACT COPYRIGHT 2005 ACS on STN

TI Preparation of axially chiral N,N'-diarylimidazolium and N-arylthiazolium salts and evaluation of their catalytic potential in the benzoin and in the intramolecular Stetter reactions

RX(1) OF 30

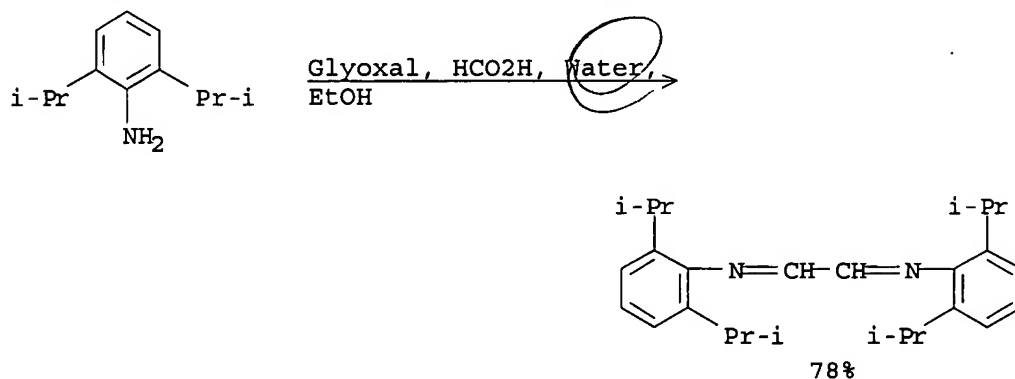


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

L77 4 ANSWERS CASREACT COPYRIGHT 2005 ACS on STN

TI Efficient Cross-Coupling of Aryl Chlorides with Aryl Grignard Reagents (Kumada Reaction) Mediated by a Palladium/Imidazolium Chloride System

RX(1) OF 16



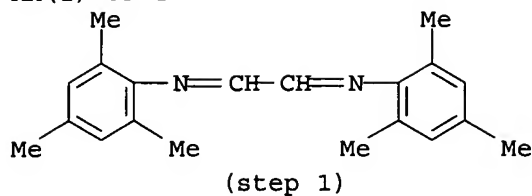
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

L77 4 ANSWERS CASREACT COPYRIGHT 2005 ACS on STN

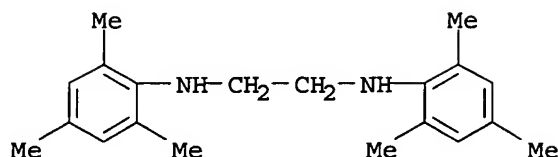
TI Imidazolylidenes, imidazolinyldenes and imidazolidines

Tetrahedron

RX(1) OF 14



1. NaBH₄, THF
 2. HCl, Water,
 F3CCO₂H



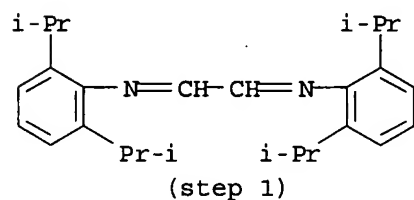
2 HCl
 85%

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

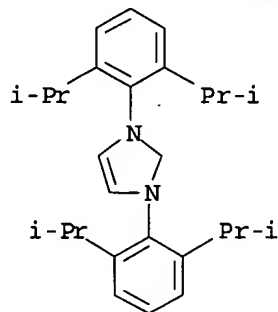
157 4 ANSWERS CASREACT COPYRIGHT 2005 ACS on STN

TI A sterically demanding nucleophilic carbene: 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene. Thermochemistry and catalytic application in olefin metathesis

RX(2) OF 15



1. HCHO, PhMe
 2. HCl, Dioxane



Cl-
 47%

NOTE: PARAFORMALDEHYDE USED

ALL ANSWERS HAVE BEEN SCANNED

=>

IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> d his

(FILE 'HCAPLUS' ENTERED AT 14:12:00 ON 24 MAR 2005)

DEL HIS
E NOLAN S/AU
L1 75 S E3,E8,E30,E32,E35,E37
L2 5 S L1 AND ?IMIDAZOL?
L3 1 S L2 AND 1 3 DISUBSTITUTED
L4 11 S 1 3 BIS 2 6 DIISOPROPYLPHENYL IMIDAZOLIUM CHLORIDE
L5 14 S 1 3 BIS 2 6 DIISOPROPYLPHENYL IMIDAZOLIUM?
L6 2 S L2 AND ?DIISOPROPYL?
L7 3 S L2 AND (1 3 OR 2 6)
L8 1 S L3 AND L6,L7
L9 3 S L6-L8
L10 2 S L9 AND BIS
SEL RN

FILE 'REGISTRY' ENTERED AT 15:01:24 ON 24 MAR 2005

L11 11 S E1-E11
L12 1 S L11 AND NCNC2/ES AND CL
L13 1 S 286014-24-2
L14 10 S 286014-24-2/CRN
L15 1 S L14 AND I
L16 2 S L12,L15
L17 1 S L11 AND C2H2O2
L18 1 S L11 AND C12H19N
L19 1 S L11 AND C26H36N2
E PARAFORMALDEHYDE/CN
L20 1 S E3
E HYDROCHLORIC ACID/CN
L21 1 S E3
E BF4H/MF
L22 1 S 14874-70-5
E TETRAFLUOROBOR/CN
E F6P/MF
L23 3 S E3
L24 7 S L11 NOT CCS/CI

FILE 'HCAPLUS' ENTERED AT 15:31:22 ON 24 MAR 2005

L25 695 S ?DIAZABUTADIEN?
L26 0 S L1 AND L25

FILE 'REGISTRY' ENTERED AT 15:32:31 ON 24 MAR 2005

L27 5 S (METHANOL OR ETHYL ACETATE OR ETHANOL OR TETRAHYDROFURAN OR T
E C20H24N2/MF
L28 153 S E3 AND 46.150.18/RID AND 2/NR
L29 3 S L28 AND BENZENAMINE AND ETHANEDIYLIDENEBIS
L30 2 S L29 AND TRIMETHYL
L31 1 S DIOXANE/CN
L32 1554 S 123-91-1/CRN
L33 5 S L32 AND CLH
L34 2 S L33 AND 2/NC
L35 3 S L11 AND NCNC2/ES NOT L12,L13
L36 1 S L35 AND C27H36N2
L37 1 S 244187-81-3/CRN
L38 1 S METHANOL/CN
L39 1 S ETHYL ACETATE/CN

FILE 'HCAPLUS' ENTERED AT 15:37:56 ON 24 MAR 2005

L40 6694 S L17
L41 11213 S GLYOXAL
L42 528 S ETHANEDIAL
L43 18 S GLYOXAZAL

L44 36 S GLYOXYLALDEHYDE
L45 12111 S L40-L44
L46 33 S L30
L47 61 S L16
L48 4 S L45 AND L47
L49 2 S L46 AND L47
L50 2 S L48 AND L49
L51 5 S L16 (L) PREP+NT/RL
L52 3 S L51 AND L45,L46
L53 1 S L1 AND L47
L54 3 S L52,L53
L55 0 S L54 AND L31,L34,L27
L56 0 S L54 AND L20-L23
L57 0 S L54 AND L27
L58 2 S L37
L59 0 S L37(L) PREP/RL
L60 8 S L10,L54,L58,L51
L61 3 S L60 AND (PY<=2002 OR PRY<=2002 OR AY<=2002)
L62 4 S L10,L61

FILE 'HCAPLUS' ENTERED AT 15:43:53 ON 24 MAR 2005

FILE 'CASREACT' ENTERED AT 15:44:41 ON 24 MAR 2005

L63 STR
L64 0 S L63
L65 STR L63
L66 8 S L65
L67 STR L63
L68 5 S L67
L69 98 S L67 FUL
SAV L69 SHIAO653/A
L70 23 S L69 AND L20-L23
L71 21 S L70 AND L27
L72 STR L67
L73 96 S L72 FUL SUB=L69
SAV L73 SHIAO653A/A
L74 23 S L73 AND L70
L75 6 S L74 AND (IMIDAZOL? OR DIARYLIMID?)/TI
L76 4 S L75 NOT (OXALA? OR OXALIC?)/TI
L77 4 S L76 AND L70,L71,L74

FILE 'CASREACT' ENTERED AT 15:53:29 ON 24 MAR 2005

=>